MATRIX-VBS: Condensing Organic Aerosols In An Aerosol Microphysics Model

Chloe Y. Gao[1,2], Kostas Tsigaridis[3,2], Susanne E. Bauer[3,2]

[1] Department of Earth and Environmental Sciences, Columbia University, New York, NY
[2] NASA Goddard Institute for Space Studies, New York, NY
[3] Center for Climate Systems Research, Columbia University, New York, NY

National Aeronautics and Space Administration
Goddard Institute for Space Studies
New York, N.Y.

Columbia University
in the City of New York

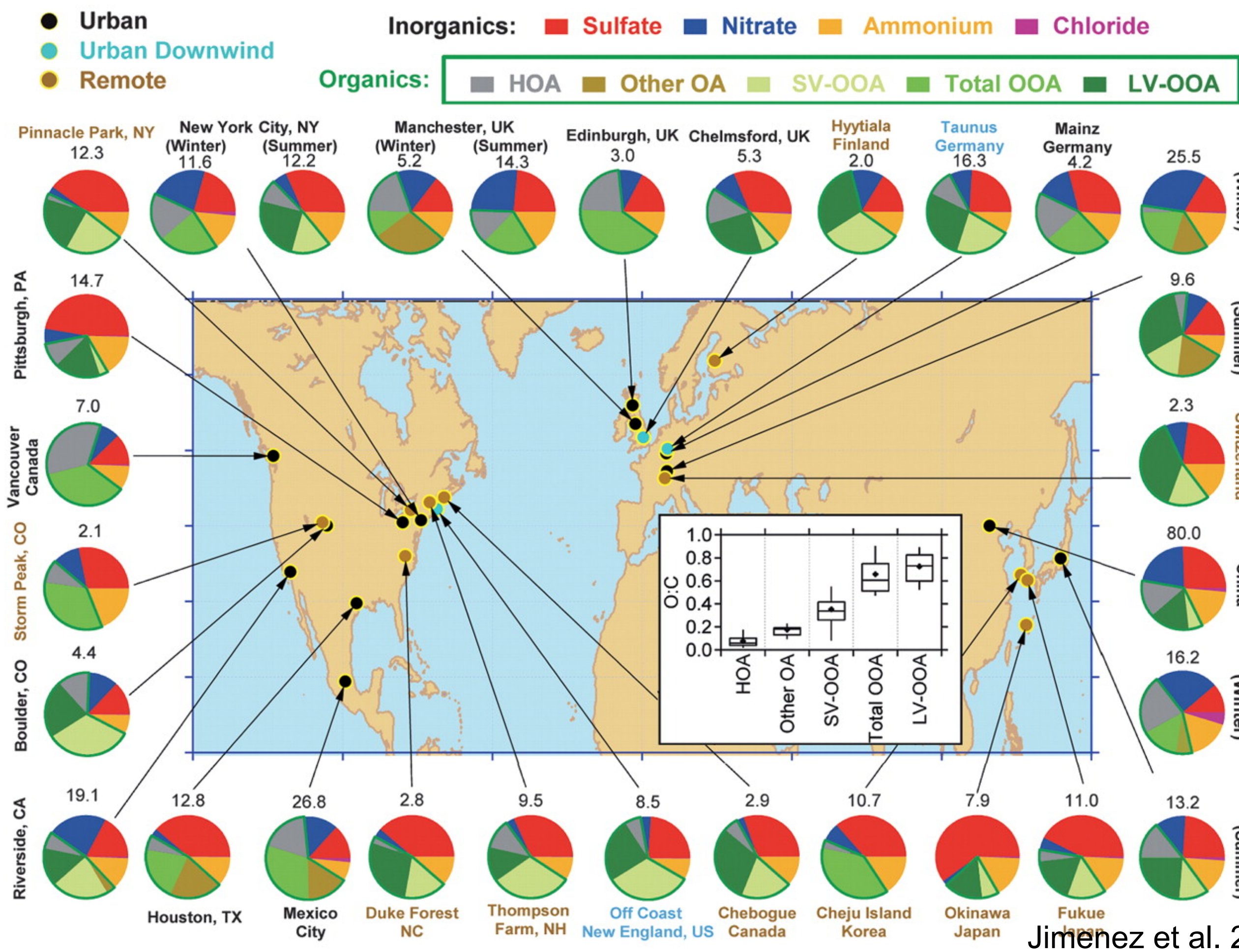
Background & Motivation

Aerosols play an important role in public health and climate.

- Organic aerosol (OA): Ubiquitous, a major component of atmospheric aerosols [*Zhang et al.* 2007]

Evolution of OA [*Jimenez et al.* 2009]:
Become more oxidized and less volatile.

HOA: surrogate for urban POA from fossil fuel burning
etc.
Other OA=other POA, e.g. BBOA
SV-OOA= semi-volatile OOA
LV-OOA=low volatility OOA
Total OOA



Jimenez et al. 2009

- **Problem:** Measurements imply that OA concentration are underestimated in models [*Tsigaridis et al.*, 2014].
- **Caused by:** missing amount organic aerosols.
- **Solution:** include semi-volatile primary organic aerosols (POA) and intermediate volatility organic compounds (IVOCs).
  - **Approach:** volatility-basis set (VBS)[*Donahue et al.* 2006]
  - **Past studies:** Regional [*Hodzic et al.*, 2010] and global [*Farina et al.*, 2010; *Jathar et al.*, 2011; *Pye and Seinfeld*, 2010; *Robinson et al.*, 2007; *Shrivastava et al.*, 2008, *Tsimpidi et al.*, 2014].

Important for aerosol size distribution:

- Very low volatility organics play a key role in particle growth: condense on all sizes.

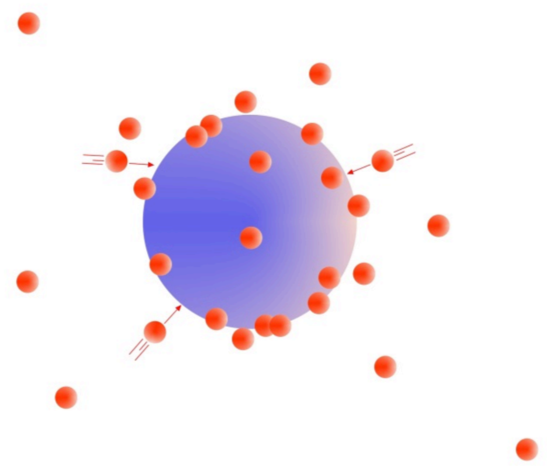
- The range of volatilities contributing to aerosol growth increases with aerosol size [*Pierce et al.*, 2011; *Yu*, 2011].

Condensation	High Volatility	Low Volatility
Small particles	no	yes
Large particles	yes	yes

- Affects aerosol size and mixing state & its impact on climate.

Objective

To introduce the process of condensing organics in an aerosol microphysics model.



Method and Approach

- Coupling the GISS ModelE2 MATRIX scheme with the VBS framework in a box model.

MATRIX

- Aerosol microphysics model, stand alone box model or module within the GCM – identical code
- Describes the mixing state of different aerosol populations[*Bauer et al.* 2008].
- POA: non-volatile
- No condensation of organics.

+

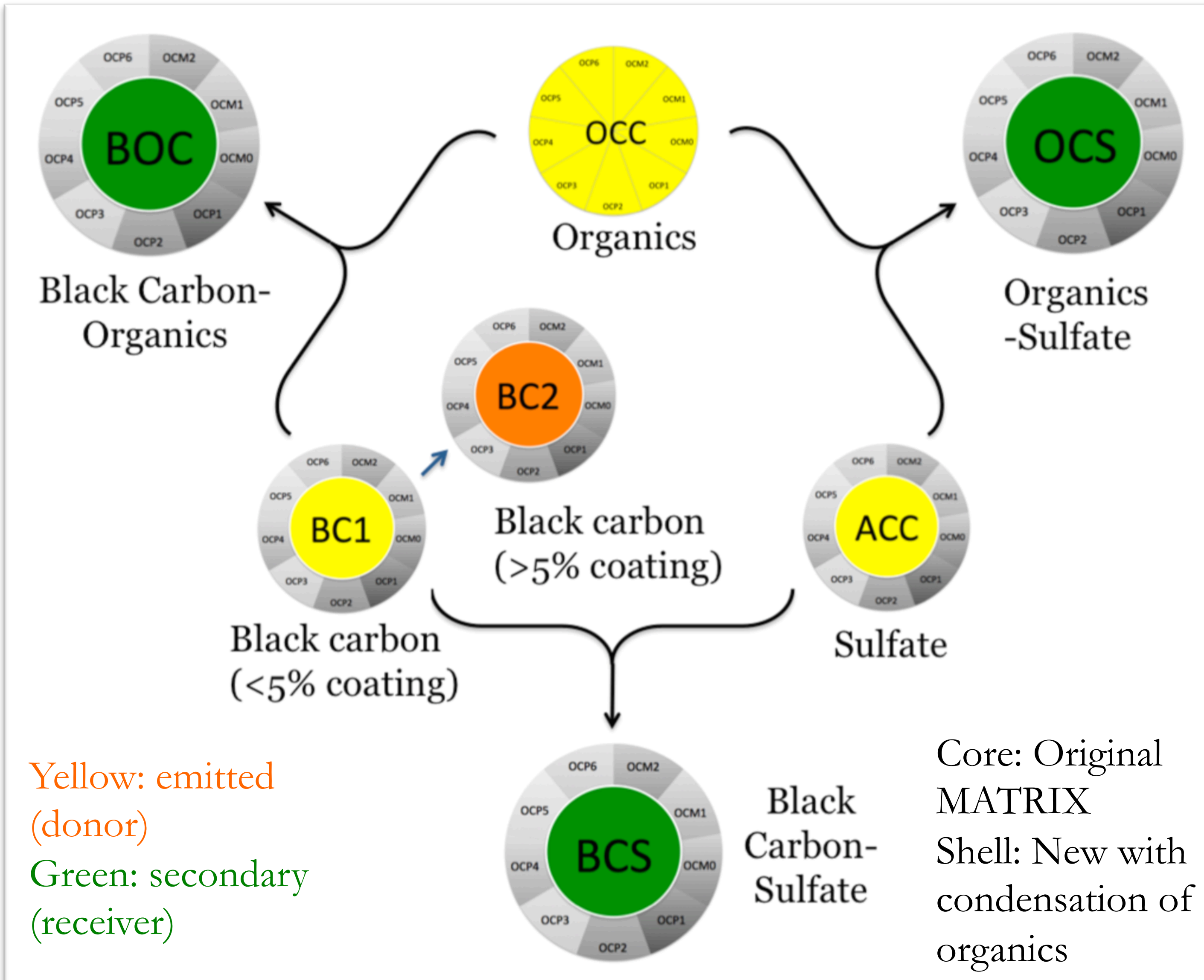
VBS

- Describes organic aerosols by separating low volatility organics into bins of effective saturation concentration, including gas-particle partition [*Donahue et al.* 2006].

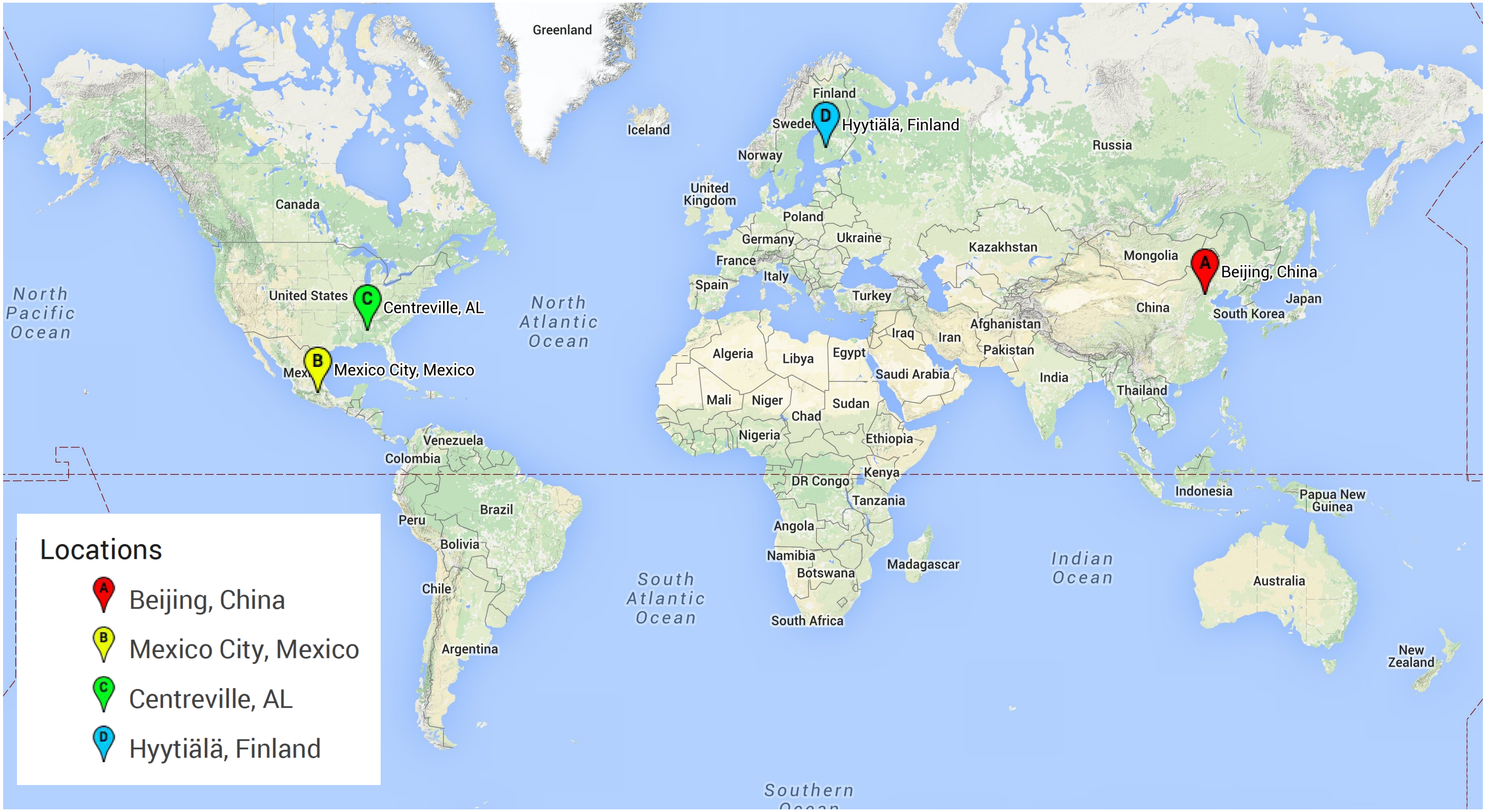
✓ **New version:**

- POA – semi-volatile, SVOCs and IVOCs represented with VBS
- Partition among different aerosol populations based on size and volatility, capturing particle growth via organic condensation

Mixing State



Case Studies



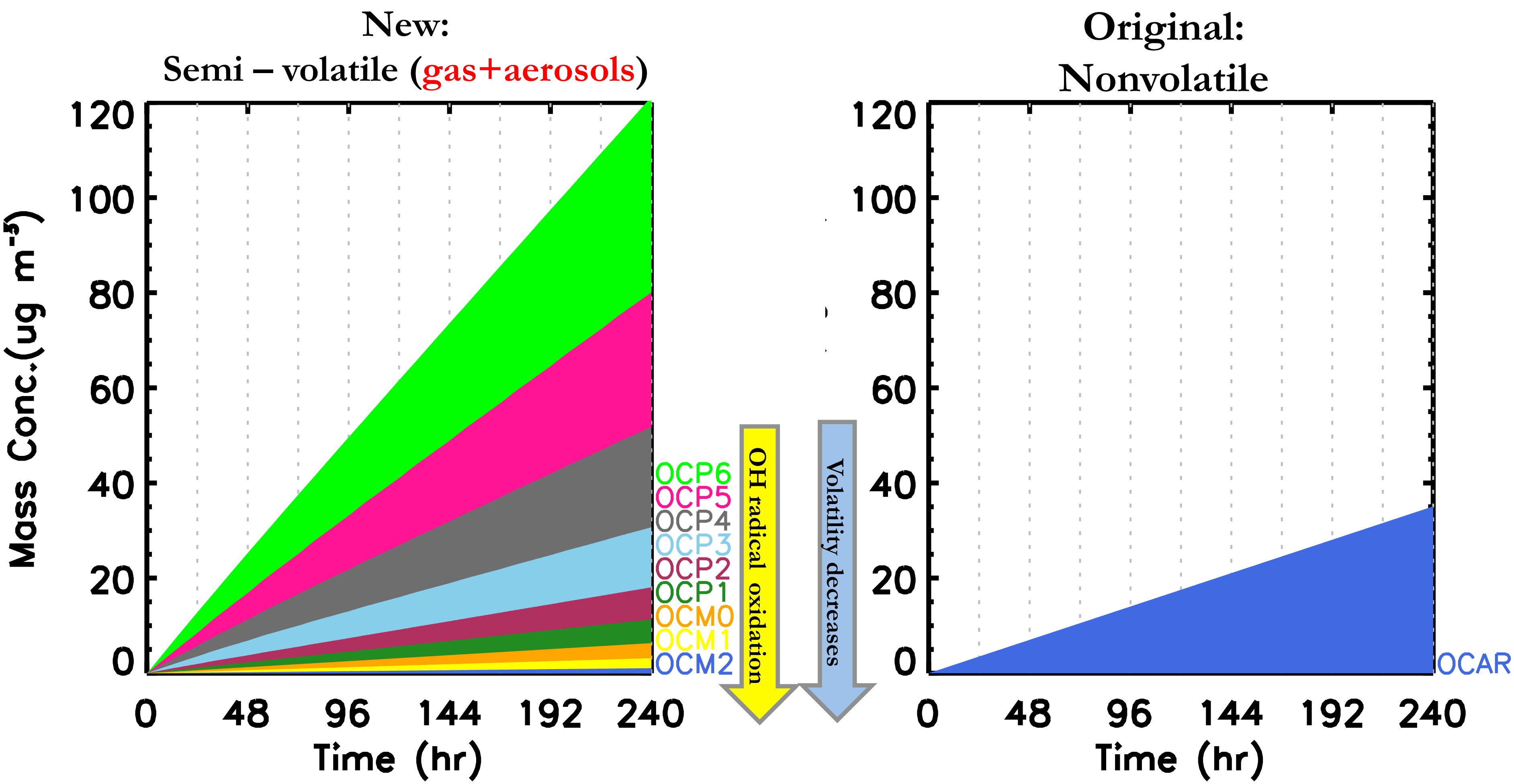
Conditions

- Duration: 10 days
- Initial conditions from global model surface values output

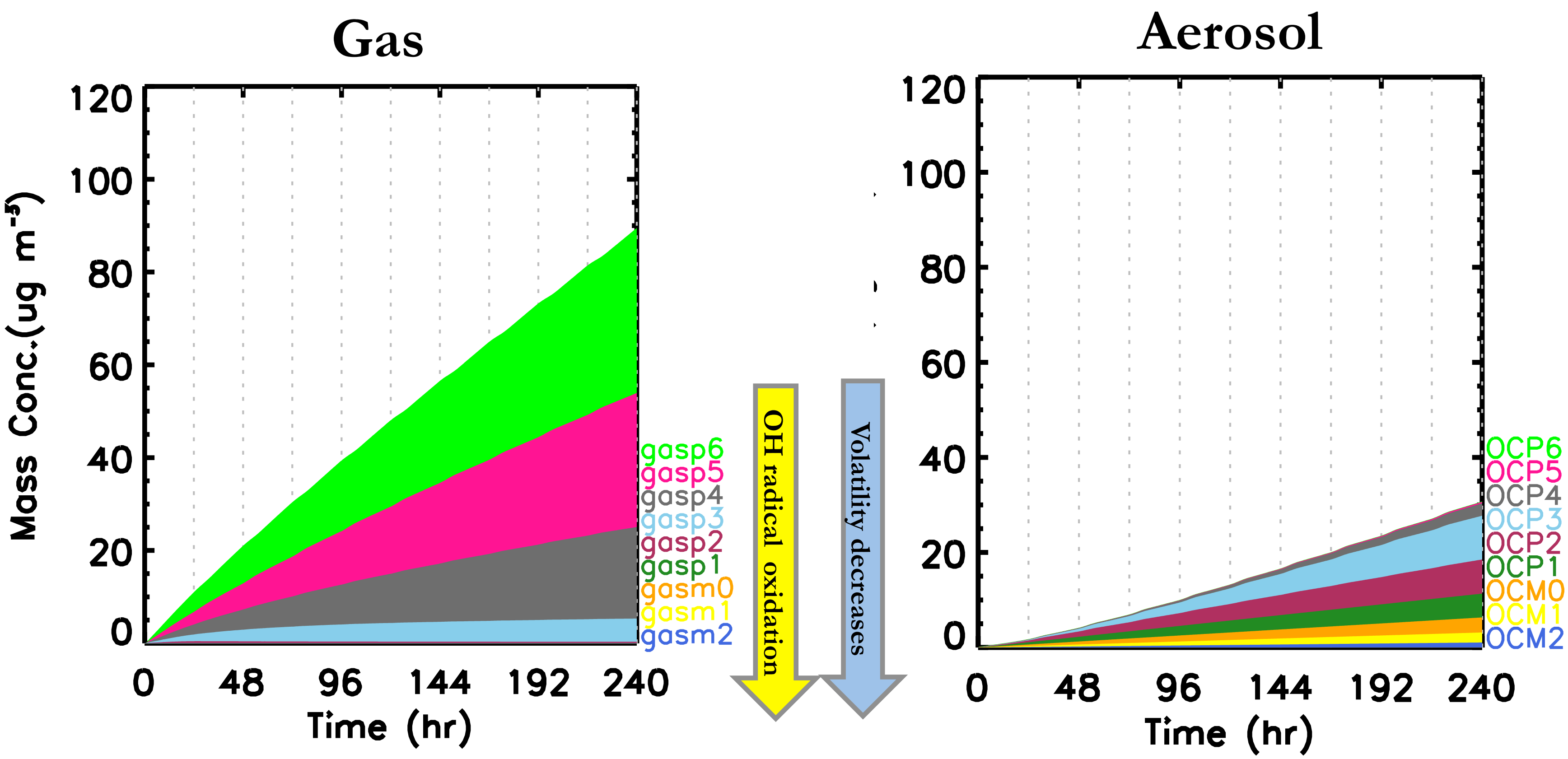
March 2006		Units	Beijing	Centreville	Hyytiälä	Mexico City
Parameters	Temperature	K	278	289	268	289
	Pressure	hPa	1005	996	1009	797
	RH	%	46.6	77.7	79.5	62.5
Gas emissions	NO_x	pptv/hr	222.2	90.3	172.0	143.1
	CO		7188.1	1383.7	570.0	2481.6
	Alkenes		4.4	0.3	0.1	1.4
	Paraffin		8.5	2.3	0.6	10.8
	Terpenes		4.1	41.6	15.2	34.5
	Isoprene		24.0	106.1	0.2	34.5
	SO_2		577.5	197.7	24.7	551.0
	NH_3		187.4	24.5	52.0	63.0
Aerosol emissions	sulfate	$ug/m^3/hr$	0.06	0.02	0.003	0.05
	black carbon		0.09	0.01	0.008	0.03
	organics*		0.19	0.03	0.015	0.11

*Organics 2.5x more in the new scheme. (*Shrivastava et al.*, 2008)

Beijing: Semi-volatile vs. Nonvolatile Organics

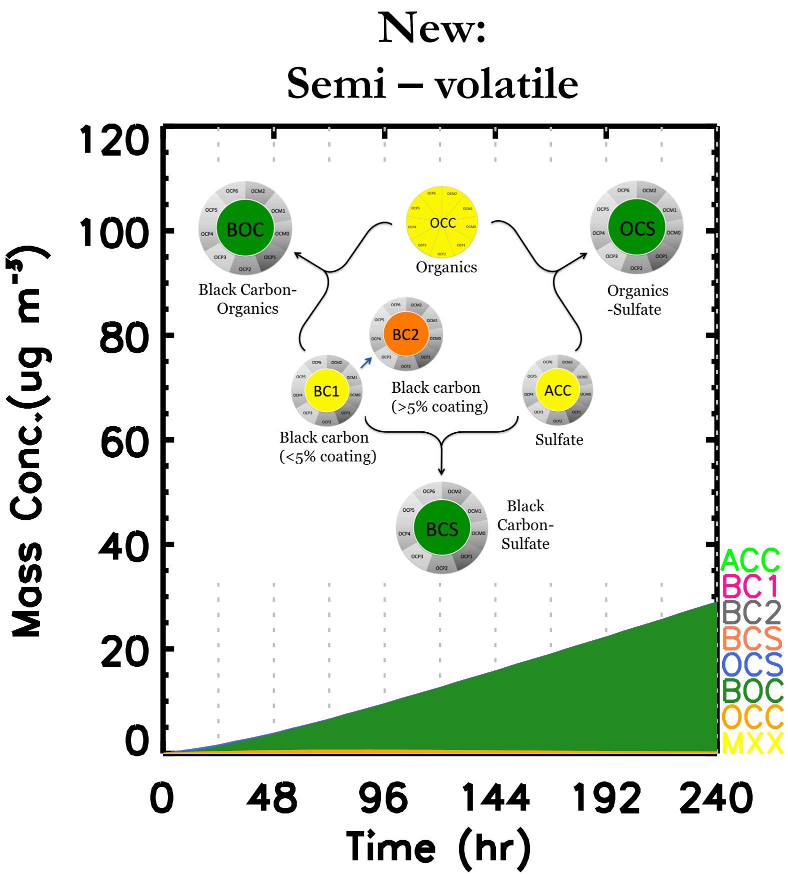


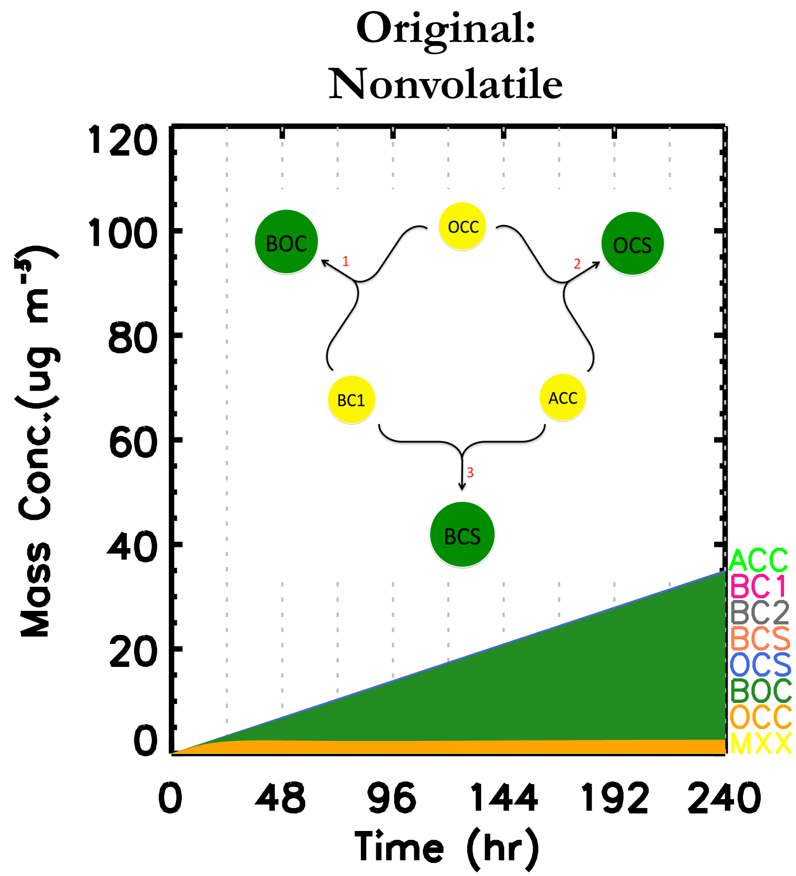
Beijing: gas phase vs. aerosol phase organics



- High volatile species in the gas phase
- Low volatile species in the aerosol phase
- Intermediate volatility bins partition between gas and aerosol phase

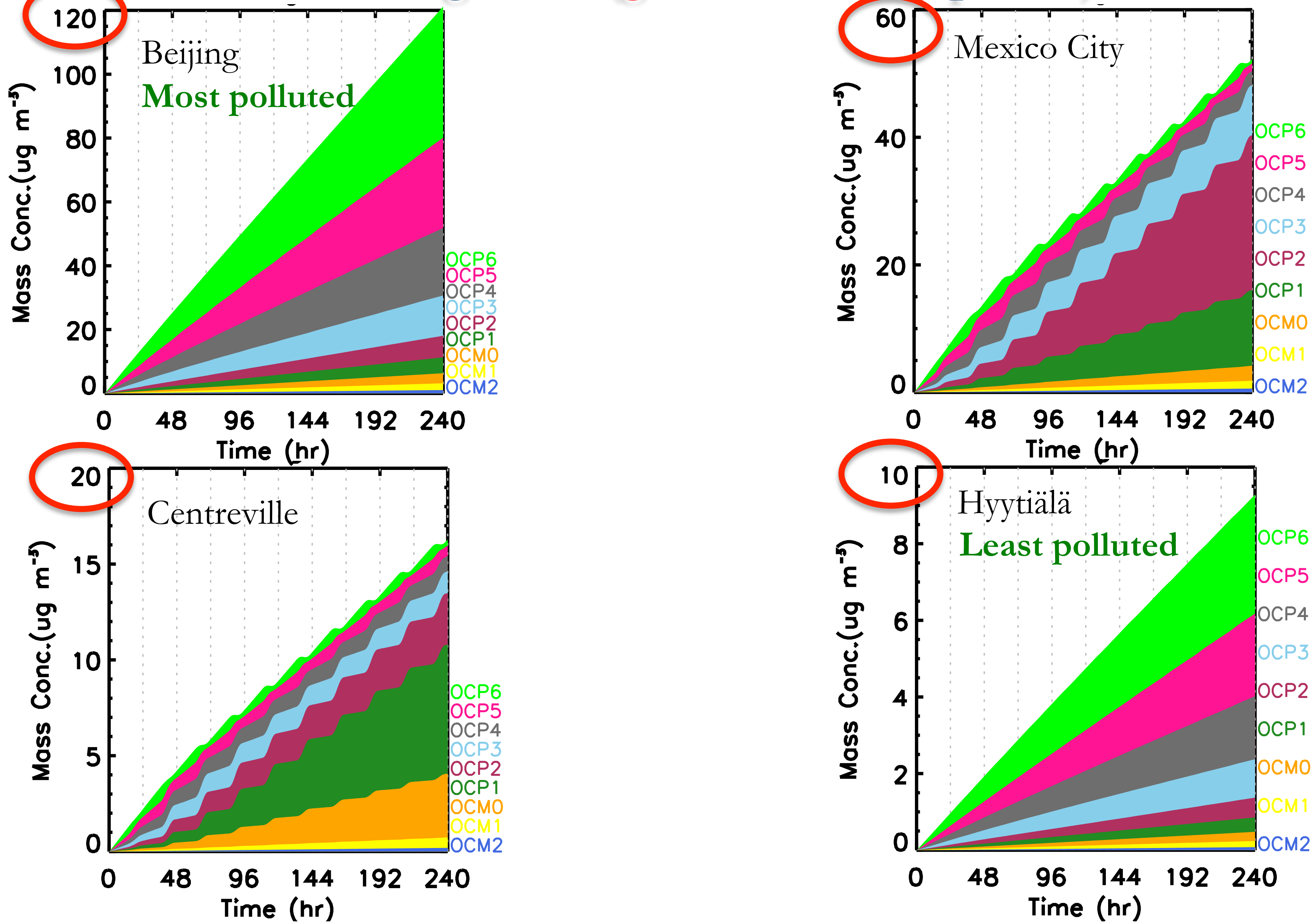
Beijing: Mixing state – organics aerosols per population



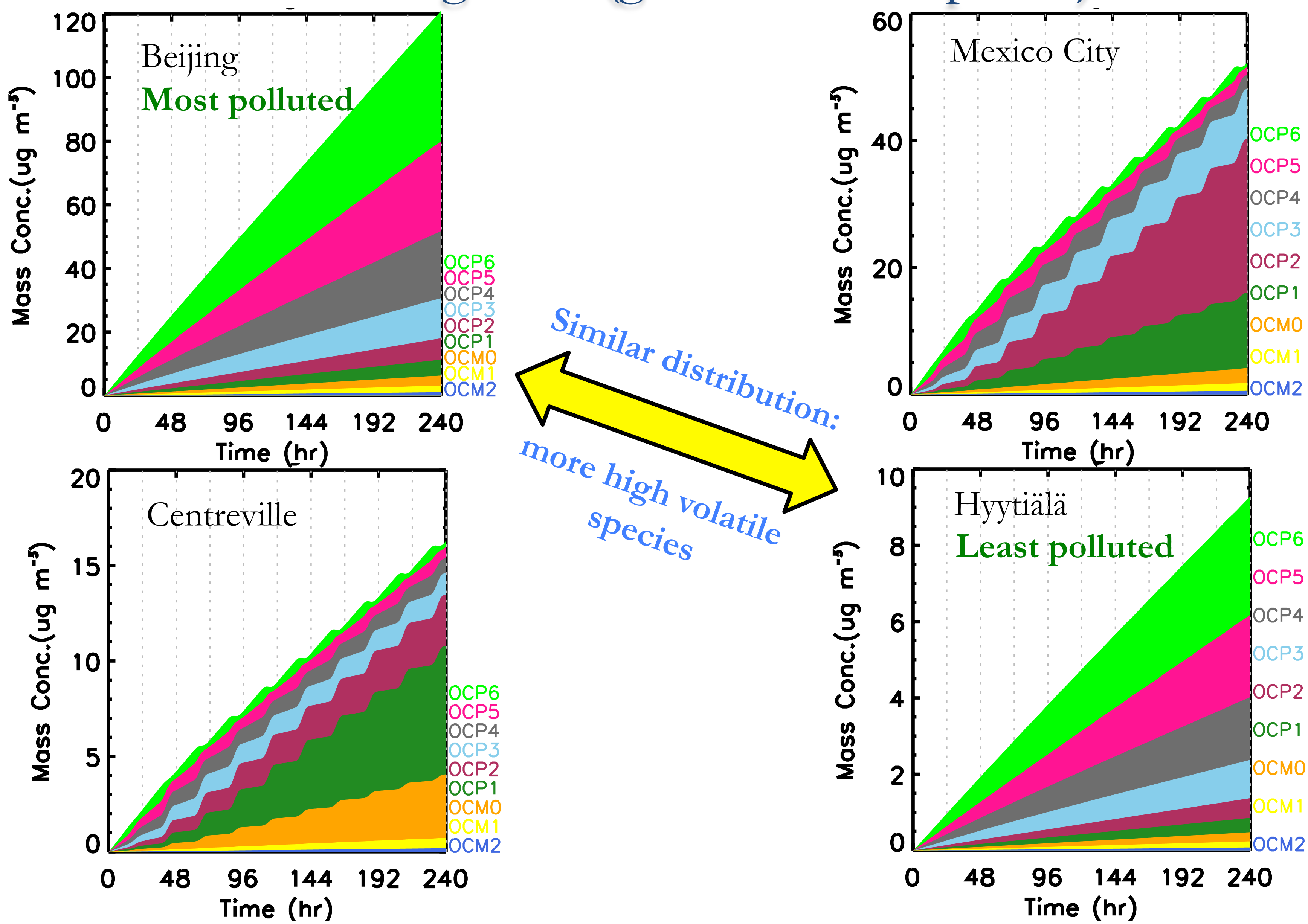


- Organics emitted in OCC – previously nonvolatile, now semi-volatile
- Difference: OA loss – previously via coagulation, now coagulation and evaporation into gas phase & condensation onto others
- Similarity: both favor BOC (more BC1 than ACC, largest surface area)

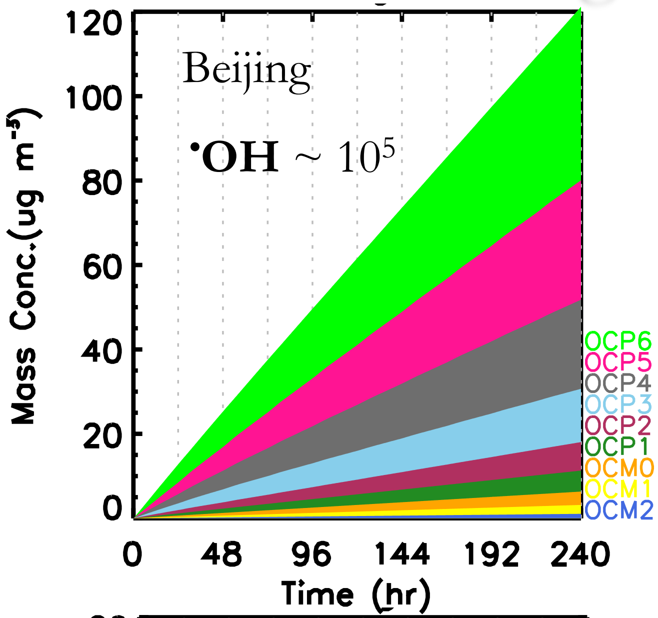
Stations Comparison:
Total Organics (gas + aerosol phase)

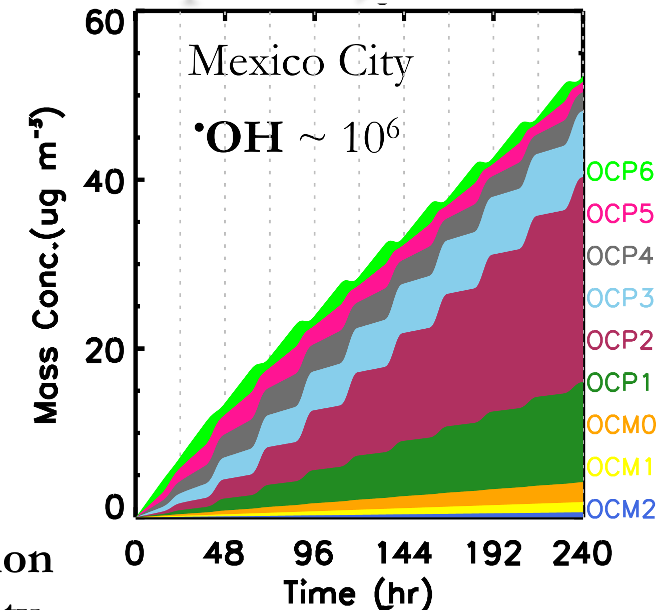


Stations Comparison:
Total Organics (gas + aerosol phase)



Stations Comparison:
Total Organics (gas + aerosol phase)

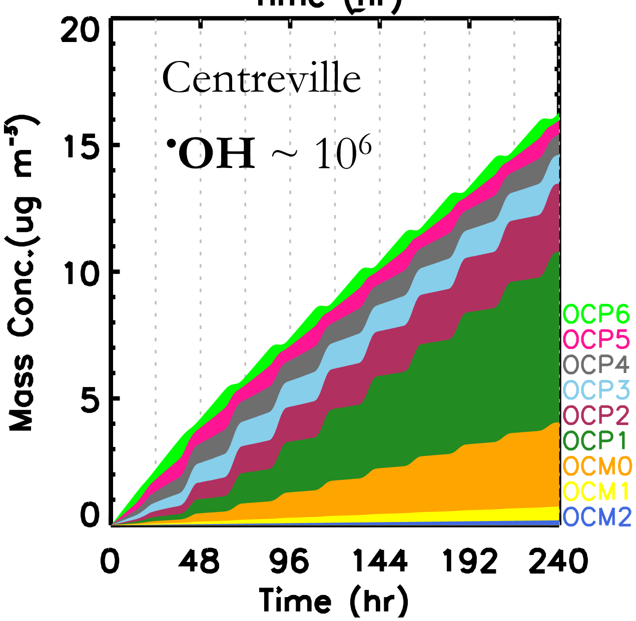


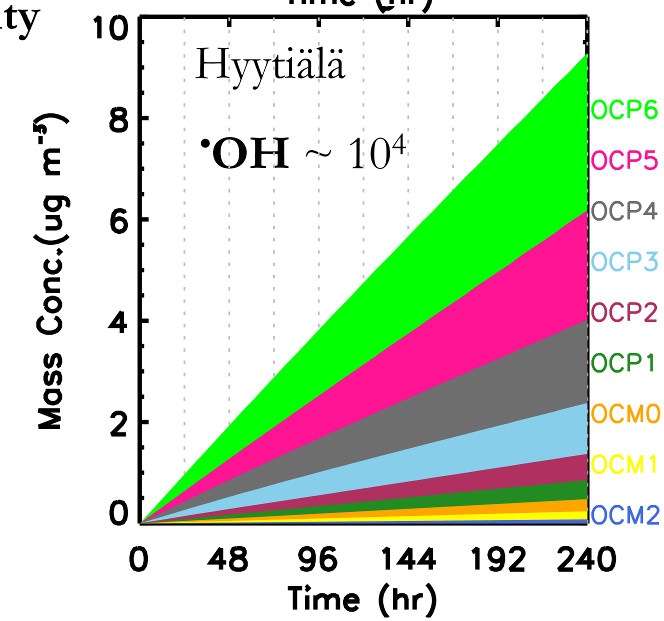


•OH determines

1) Oxidation – volatility distribution

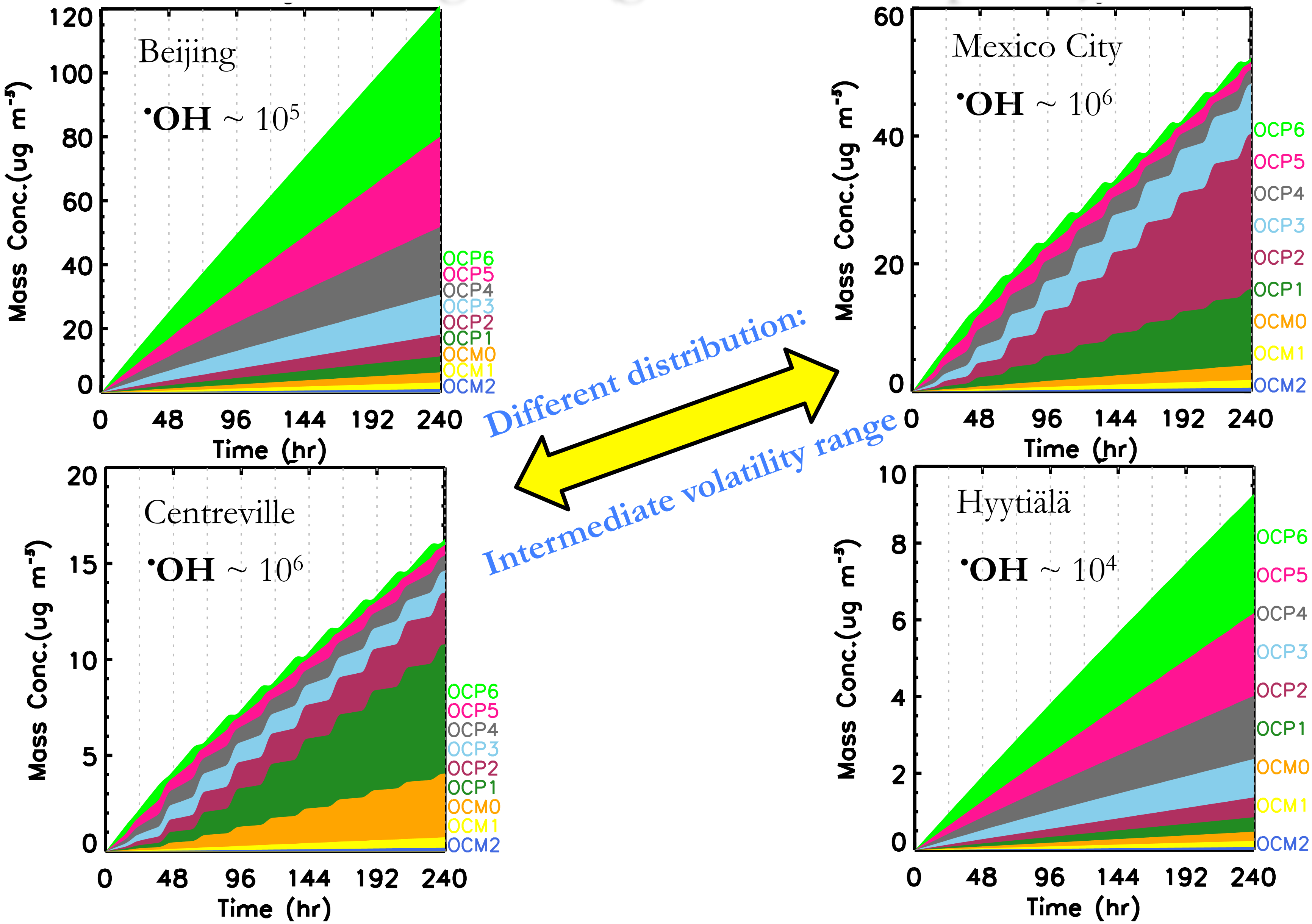
2) Diurnal variability





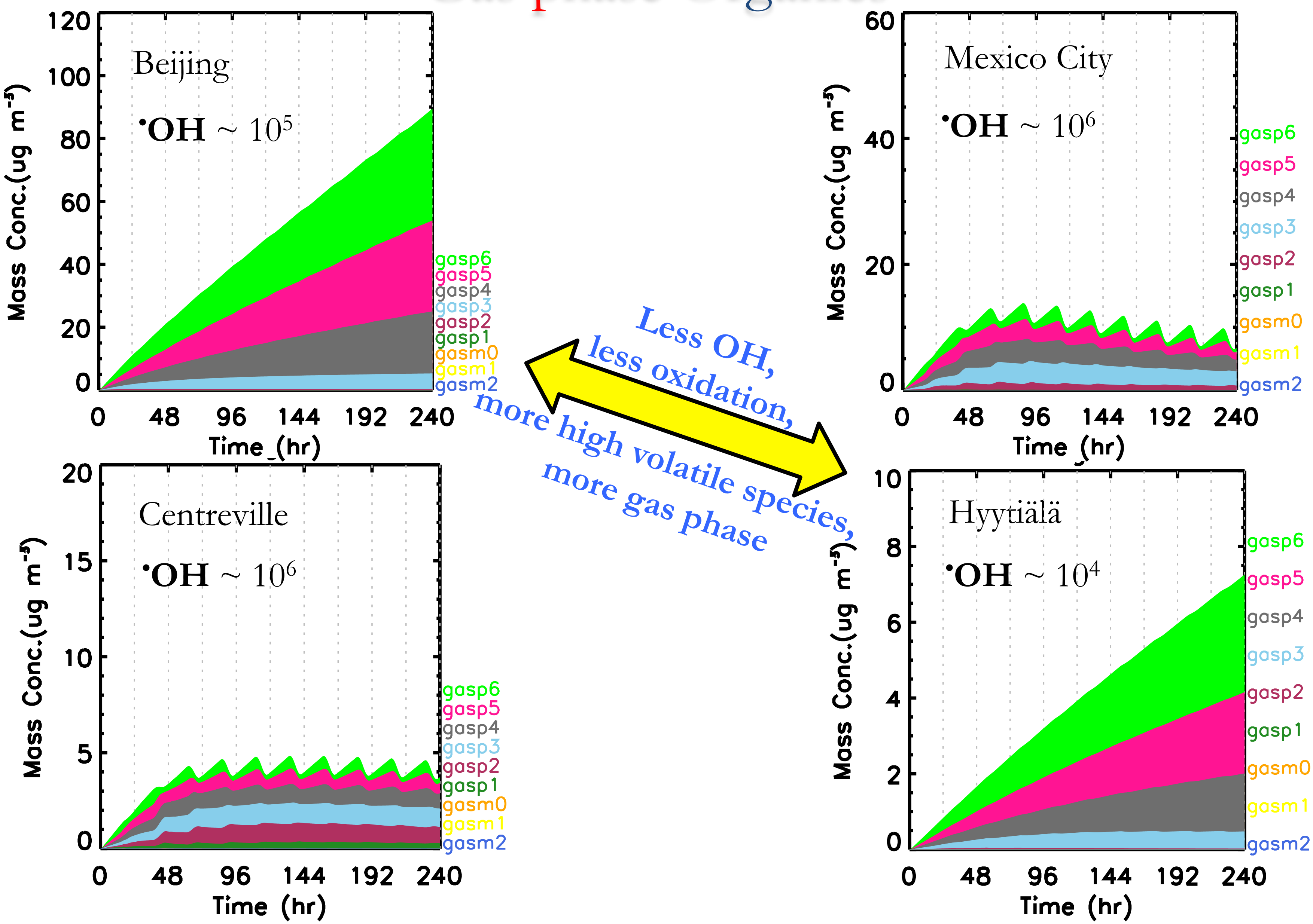
Stations Comparison:

Total Organics (gas + aerosol phase)



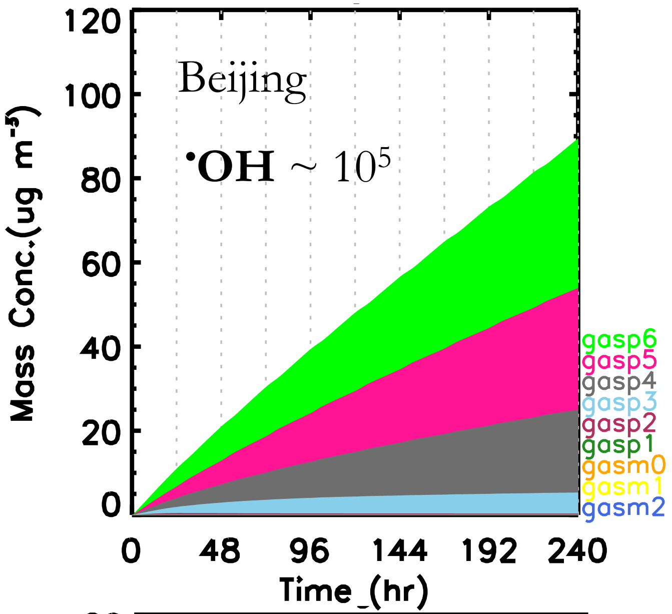
Stations Comparison:

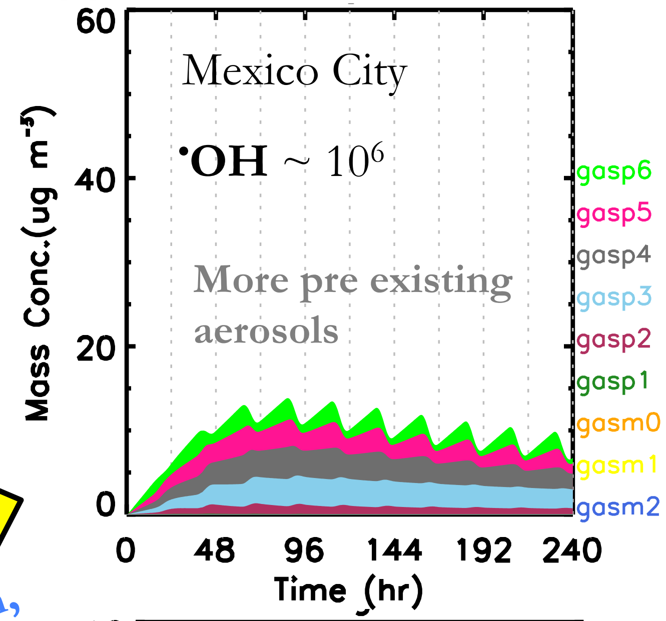
Gas phase Organics



Stations Comparison:

Gas phase Organics

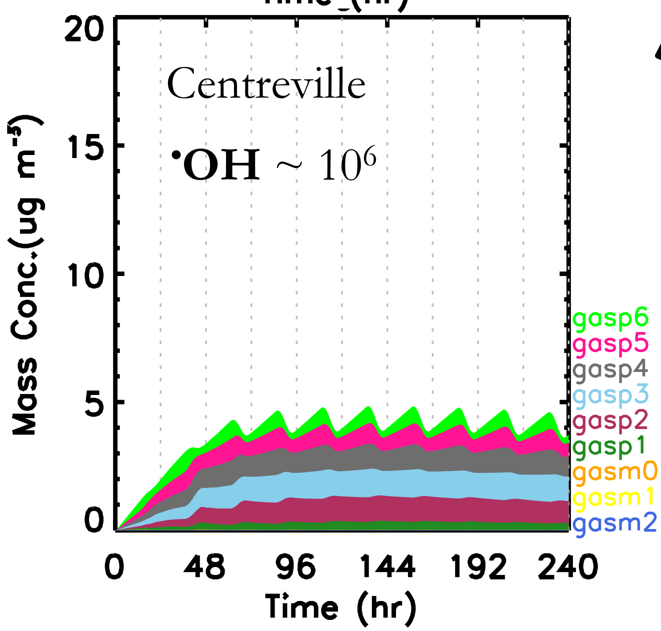


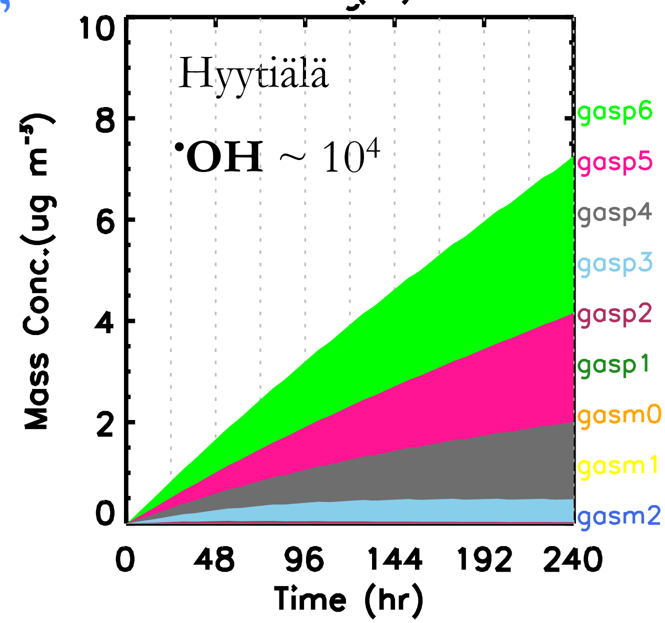


Similar OH,

one ~equilibrium,

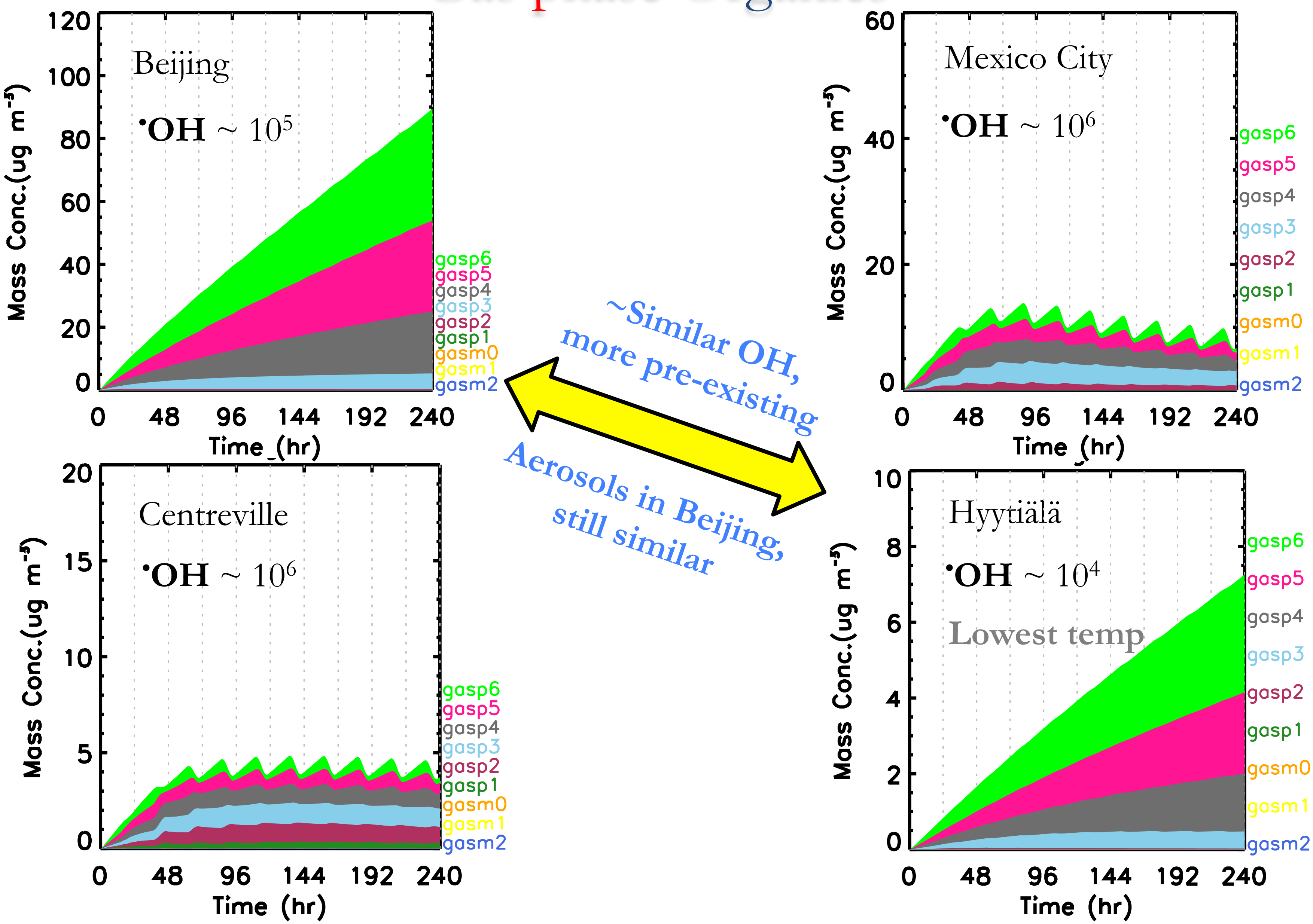
one decreases





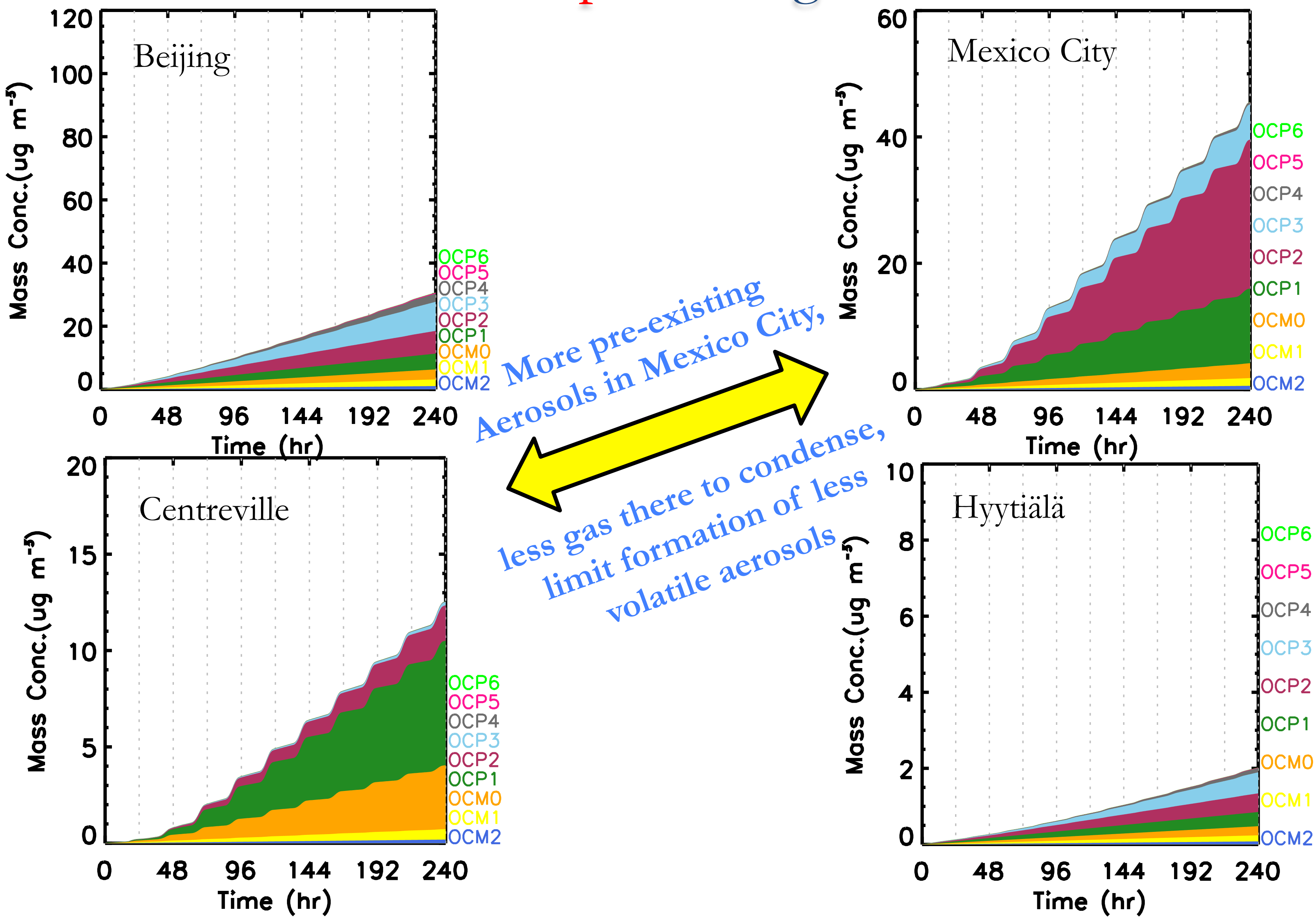
Stations Comparison:

Gas phase Organics



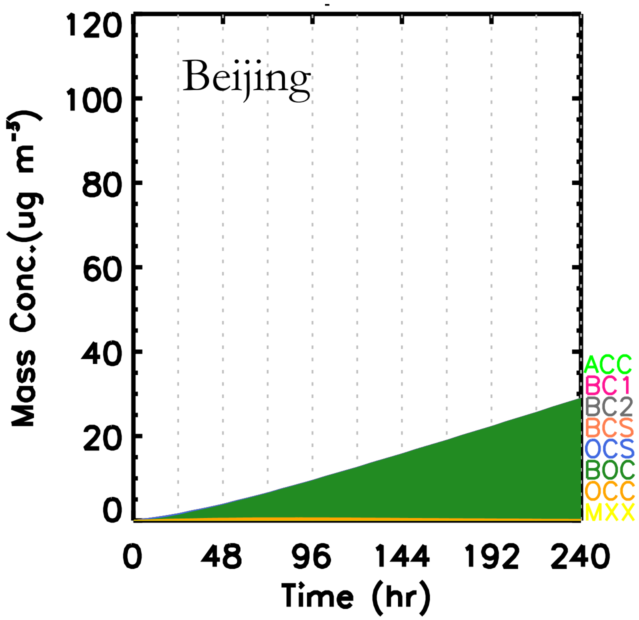
Stations Comparison:

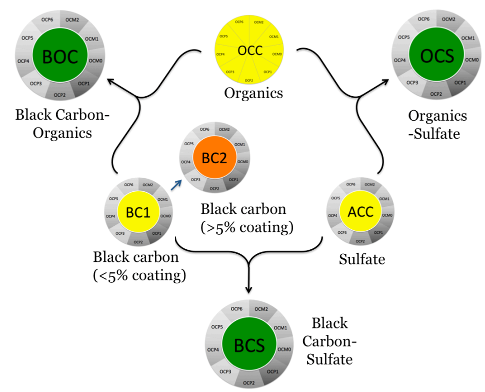
Aerosol phase Organics

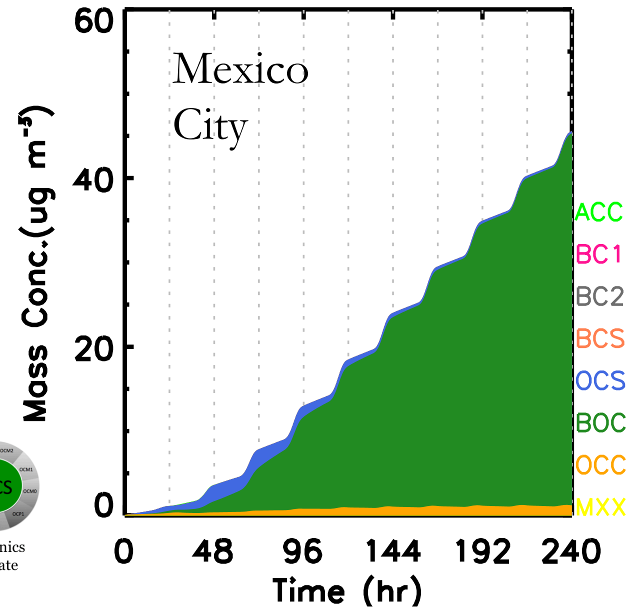


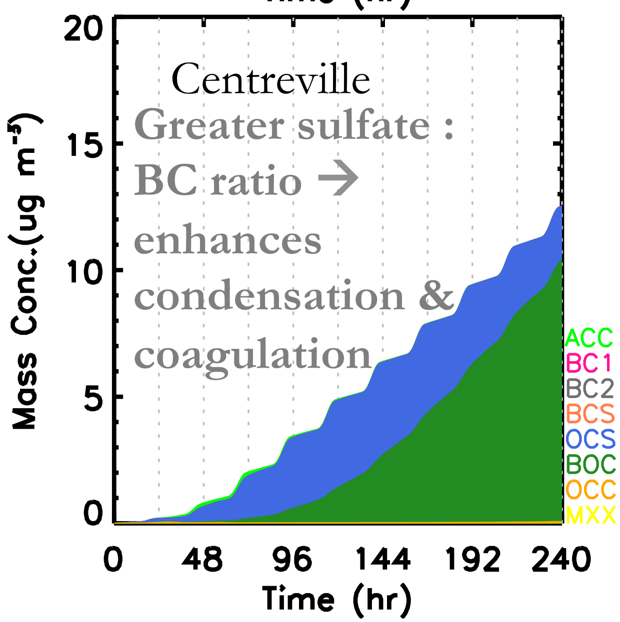
Stations Comparison:

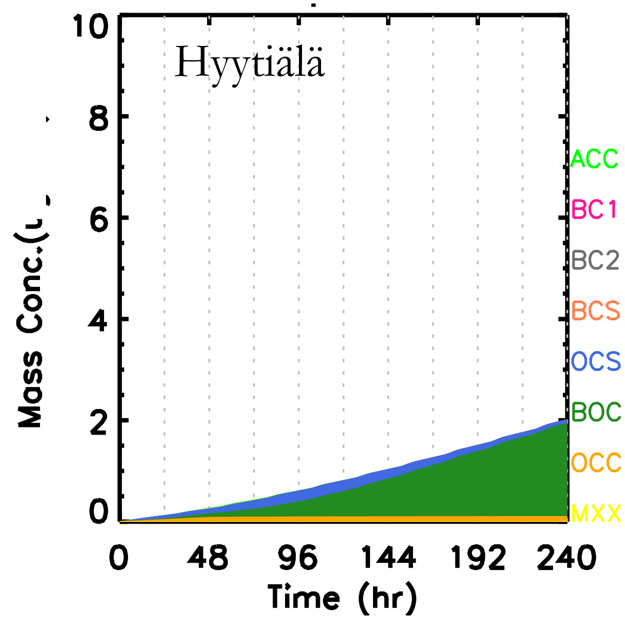
Mixing State











Conclusion

- Beijing and Hyytiälä
  - Different pollution levels, similar distribution of volatility & mostly in the gas phase due to low $^{\bullet}OH$ levels
  - Different amount of pre-existing aerosols, still similar distribution due to different temperatures

- Mexico City and Centreville
  - Similar $^{\bullet}OH$ levels, different distribution of volatility due to different amount of pre-existing aerosols
  - More $^{\bullet}OH$ than in Beijing and Hyytiälä, mostly in the aerosol phase

Future Work

- ✓ Stage 1: Box model development
- ✓ Stage 2: Case Studies
- ❑ Stage 3: Sensitivity tests & include condensing organics in dust and sea salt aerosols
- ❑ Stage 4: Simplification: Reduce number of tracers
- ❑ Stage 5: GCM implementation: box model is a module within GISS ModelE2 – identical code